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Coarse-grained models for biological simulations ZHE WU, QIANG CUI, ARUN YETHIRAJ, UW Madison — The large timescales and length-scales of interest in biophysics preclude atomistic study of many systems and processes. One appealing approach is to use coarse-grained (CG) models where several atoms are grouped into a single CG site. In this work we describe a new CG force field for lipids, surfactants, and amino acids. The topology of CG sites is the same as in the MARTINI force field, but the new model is compatible with a recently developed CG electrostatic water (Big Multiple Water, BMW) model. The model not only gives correct structural, elastic properties and phase behavior for lipid and surfactants, but also reproduces electrostatic properties at water-membrane interface that agree with experiment and atomistic simulations, including the potential of mean force for charged amino acid residuals at membrane. Consequently, the model predicts stable attachment of cationic peptides (i.e., poly-Arg) on lipid bilayer surface, which is not shown in previous models with non-electrostatic water.

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